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July 1, 1993

Professor Lederberg
Rockefeller University
1230 York Avenue
New York, NY 10021

Dear Professor Lederberg:

I am attempting to write a program to calculate possible molecular formulas from a supplied molecular weight. I have a copy of your 1964 NASA article outlining an algorithm and tables for doing that. To date, I have not been able to find many references, other than your article, for making such calculations.

What I am really interested in is an algorithm for making *ab intio* calculations, without the use of tables. I would be grateful if you could send me references to any publications dealing with calculating molecular formulas from either high resolution mass spectral data or from a low resolution mass spectrum and perhaps a user-supplied number of carbons. At this point, I am interested in any and all information that is in the public domain. I program mainly in C, but could probably translate from Pascal or Fortran if I had to.

Any help you could give me would be appreciated. Thank you.

Sincerely,

James Deline

JUL - 8 1993

What a nostalgiquic request.
The computers are so cheap + fast now that most people just do it by brute force with a set of nested for loops ranging over plausible numbers of C, N, O ... But you may want to use the strategies in the method. If you do make a "C version" I'd be grateful for a copy. The ancient Fortran is lost.

Sincerely.

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